Shell model on a random gaussian basis

K. Varga
Institute of Nuclear Research of the Hungarian Academy of Sciences
(MTA ATOMKI) Debrecen, Hungary
and
R.J. Liotta
Royal Institute of Technology, S-10405 Stockholm, Sweden

February 9, 2008

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Abstract

Pauli-projected random gaussians are used as a representation to solve the shell model equations. The elements of the representation are chosen by a variational procedure. This scheme is particularly suited to describe cluster formation and cluster decay in nuclei. It overcomes the basis-size problem of the ordinary shell model and the technical difficulties of the cluster-configuration shell model. The model reproduces the α-decay width of ^{212}Po satisfactorily.

1 Introduction

By complementing the shell model with a cluster-model basis, the α-decay of ^{212}Po can be described very well [1]. This cluster-configuration shell model or hybrid model is, however, difficult to apply. We have therefore developed a simpler model which is closer to the conventional shell model but in practical

applications may prove to be far superior. The objective of this paper is to report on this new model and its performance in the calculation of the ground state of ^{212}Po. To this end, we compare its results with those of the hybrid model [1].

The new model is essentially a shell model, in which the valence orbits are replaced by combinations of gaussian functions of different size parameters, with exact Pauli projection off the core orbits. These gaussians are more flexible than the harmonic oscillator single-particle (s.p.) functions because their width parameters are free. A variational backgroud can guarantee that they will be automatically chosen so as to suit to the problem considered. In particular, the gaussians can produce a more realistic fall-off in the surface, which is important for the description of decay processes. Moreover, in the interior the gaussians are able to simulate the effects of several oscillator shells. Note that the Pauli projection provides the gaussians with some, say n_0, nodes, so that n gaussians in the expansion of a s.p. function will involve s.p. orbits of $n_0, \ldots, n_0 + n - 1$ nodes. In spite of the inclusion of such high-lying shells, the problem may still remain tractable if the basis elements are carefully selected. We admit states in the basis depending on their contribution to the g.s. energy. This method of choosing random states as candidates for the basis is called [2] "stochastic variational method".

2 The formalism

The basic building block of our s.p. basis is the gaussian (or nodeless harmonic oscillator function) of size parameter ν, defined by

$$\varphi_l^\nu(r) = \left(\frac{2^{l+2}(2\nu)^{l+3/2}}{\sqrt{\pi}(2l+1)!!} \right)^{1/2} r^l e^{-\nu r^2}. \tag{1}$$

As any well-behaved function can be approximated with any prescribed precision by a linear combination of gaussians of different size parameters, $\sum_i c_i \varphi_l^{\nu_i}(r)$, one can use such combinations to approximate the valence s.p. functions of the shell-model Hamiltonian.

These gaussians are not orthogonal to the core orbits. To take care of antisymmetrization, one can introduce the operator that projects out the s.p.

states occupied in the core [1, 3]:

$$P_i = 1 - \sum_{j=5}^{A} |\phi^j(i)\rangle\langle\phi^j(i)| \tag{2}$$

The index i distinguishes the proton ($i = 1, 2$) and neutron ($i = 3, 4$) orbits.

The Pauli-correct s.p. wave functions are then constructed as

$$\hat{\varphi}^{\nu}_{lj}(i) = P_i \left\{ \varphi^{\nu}_{l}(r_i) \left[Y_l(\hat{r}_i)\chi_{\frac{1}{2}}(i) \right]_{jm} \right\} \tag{3}$$

where $\chi_{\frac{1}{2}\sigma}(i)$ is the spin function of the ith nucleon.

In the description of ^{212}Po it is reasonable to assume the core, ^{208}Pb, to be passive and massive. (This approximation could be removed by using the formalism of the cluster-orbital shell model [4].)

As these s.p. functions are fully analogous to those in the conventional shell model, the many-particle basis can be constructed in the usual way. In proton-neutron formalism and jj coupling scheme the two-proton and two-neutron functions are given by

$$\Psi^i_{\pi} = \mathcal{A} \left[\hat{\varphi}^{\nu^i_1}_{l_1 j_1}(1) \hat{\varphi}^{\nu^i_2}_{l_2 j_2}(2) \right]_{J_\pi} \tag{4}$$

and

$$\Psi^j_{\nu} = \mathcal{A} \left[\hat{\varphi}^{\nu^j_3}_{l_3 j_3}(3) \hat{\varphi}^{\nu^j_4}_{l_4 j_4}(4) \right]_{J_\nu}, \tag{5}$$

where the operator $\mathcal{A}$ antisymmetrizes between like particles, $\pi = \{l_1, j_1, l_2, j_2, J_\pi\}$, $\nu = \{l_3, j_3, l_4, j_4, J_\nu\}$. A four-particle state is formed as

$$\Psi^k_{(\pi\nu)JM} = \left[\Psi^i_{\pi} \Psi^j_{\nu} \right]_{JM}. \tag{6}$$

The trial function is then

$$\Psi_{JM} = \sum_{\pi\nu k} c_k \Psi^k_{(\pi\nu)JM}. \tag{7}$$

To describe the dynamics of the valence particles, we minimize the expectation value of their Hamiltonian

$$H = \sum_{i=1}^{4} (T_i + U_i) + \sum_{1 \le i < j \le 4} V_{ij}, \tag{8}$$

where T is the kinetic energy, U is the core-particle interaction and V is the particle-particle interaction.

The trial function Ψ_{JM} contains a great number of terms belonging to different configurations and size parameters. Since the dependence of the eigenvalue problem upon the variational parameters c_i is linear one can determine them by finding the lowest eigenvalue of a generalized linear algebraic eigenvalue problem, i. e.

$$\mathbf{Hc} = E_N \mathbf{Ac}, \tag{9}$$

where $\mathbf{H}$ and $\mathbf{A}$ are the Hamiltonian and overlap matrices. The subscript N stands for the dimension of the eigenvalue problem. The overlap matrix $\mathbf{A}$ is nondiagonal due to the nonorthogonality of the functions $\Psi^k_{(\pi\nu)JM}$.

This variational approach is only expected to yield a good approximation to the g.s. energy if the size parameters $\nu_1^k, ..., \nu_4^k$ are adequately chosen. Previous experience with the stochastic multicluster model [2] shows that the number of basis states needed is not excessive even in the five-cluster case, which is comparable with the present core plus four-nucleon system.

We generated trial basis states randomly, and singled out, by an admittance test, the ones whose contribution to the g.s. energy was larger than a preset limit, ε ("utility testing" [2]). That is, we start (k=1) by making a random choice of the size parameter quartet $\nu_1^k, ..., \nu_4^k$ from the physically important ν region, and set up a basis state of a particular configuration. The energy expectation value gives the first approximate energy, E_1. Then we generate a new random set $\nu_1^2, ..., \nu_4^2$, and solve eq. (9) for $N = 2$. Due to the variational character of the method any parameter quartet improves the energy ($E_2 < E_1$), but we only adopt the basis element if $E_1 - E_2 > \varepsilon$. This procedure is then repeated with new random elements up to convergence, and then the basis is enlarged by including further configurations.

At each trial step the energy can be determined by solving the eigenvalue problem using any conventional numerical algorithm. But as we are only interested in the g.s. energy, and we proceed stepwise, we can use the much more economical modified Jacobi method [5]. The Jacobi method (see e. g. Ref. [6]) solves the eigenvalue problem $\mathbf{HC} = E\mathbf{C}$ eliminating the nondiagonal elements by successive plane rotations. In the modified Jacobi method, the lowest eigenvalue is only determined by elimination of the nondiagonal elements corresponding to that eigenvalue [5]. Thus it uses, in every step, the results of the diagonalization of the previous step. Although the modi-

fied Jacobi method can be generalized to solve fully the eigenvalue problem [5], we found it more convenient to re-orthogonalize our basis in each step of the random search procedure. This is advantageous because **A** is block-diagonal (each configuration provides a block) and we need to orthogonalize only within the configuration whose basis is being enlarged. Since the number of basis states in any configuration is low, this re-orthogonalization requires almost no computational effort.

A delicate point of this procedure is the choice of ε because a too large value bogs down the procedure, whereas a too small value results in highly redundant bases of large dimensions. It is expedient [5] to re-adapt the acceptance criterion dynamically. For instance, in the present calculation we started with $\varepsilon = 0.01$ MeV, and after 10 failed attempts to find a good enough basis state, we reduced ε by 2, and this was repeated two more times. In this way we managed to find further states of some significance. This procedure has been thorougly tested [2], and it was found that it is extremely powerful and reliable [2].

3 Details

The s.p. potentials include scalar and spin-orbit Woods-Saxon parts as well as the Coulomb interaction. To facilitate the analytical calculation of the matrix elements, all potential terms are expanded in terms of gaussians. To be able to compare the "pure shell model"[1] with the present model, we use the potential parameter set B of ref. [1] and employ the same Pauli projector as there, that is the occupied s.p. states are represented by oscillator functions of size parameter $\nu_0 = 0.083\text{fm}^{-2}$.

For the valence orbits we selected the size parameters from the physically important interval 4 fm $\leq \nu^{-1/2} \leq$ 14 fm. The following s.p. quantum numbers were used:

$$\begin{aligned} l, j &= h_{9/2}, f_{7/2}, i_{13/2}, f_{5/2}, p_{3/2} \quad (protons) \\ &= g_{9/2}, i_{11/2}, j_{15/2}, d_{5/2}, s_{1/2}, g_{7/2} \quad (neutrons). \end{aligned}$$

Just as in the former model, we set up the four-particle basis by coupling all possible two-particle combinations up to $J_\pi = 8$ and $J_\nu = 8$.

We build up the basis by the method skecthed above in each configuration $\{\pi\nu\}$. We ordered the configurations according to their expected

contributions to the energy, i.e. according to the sums of the s.p. energies involved and, among states involving the same s.p. states, to the two-particle angular momenta in increasing order. Thus we begin with the configurations $[[h_{9/2}]^2_{J_\pi}[g_{9/2}]^2_{J_\nu}]_0$, with $J_\pi = J_\nu = 0, 1, 2, \ldots$, $[[h_{9/2}]^2_{J_\pi}[i_{11/2}]^2_{J_\nu}]_0$, with $J_\pi = J_\nu = 0, 1, 2, \ldots$, $[[f_{7/2}]^2_{J_\pi}[g_{9/2}]^2_{J_\nu}]_0$, with $J_\pi = J_\nu = 0, 1, 2, \ldots$ etc. If a configuration cannot contribute to the g.s. energy by at least $\varepsilon/2^3$, then it is omitted.

4 Results

First we solved the eigenvalue problem of the s.p. part of the Hamiltonian on the basis (3), The scalar depth was adjusted so as to best reproduce the experimental s.p. energies, as done in ref. [1]. We obtained this with the scalar strengths $V_p = 61.60$ MeV and $V_n = 43.80$ MeV for protons and neutrons, respectively. The resulting s.p. energies are in excellent agreement with the ones obtained by a direct numerical integration.

We then calculated the g.s. ($J = 0$) energy of ^{212}Po. We terminated the random search at a basis dimension $N = 397$ and a number of configurations $n = 118$. As the number of basis states is increased the g.s. energy converges to $E = -19.25$ MeV (the experimental value is -19.35 MeV.), as seen in figure 1. This may be compared with the value $E = -18.96$ MeV of the pure shell model or the value $E = -19.18$ MeV in the hybrid model [1].

To check the convergence we repeated the calculation using different random parameter sets with dimensions $N = 413$, $n = 120$ and $N = 380$, $n = 127$. The three energies agree within 0.04 MeV. To see the role of the order of the configurations, we repeated again the calculations with reversed order. The resulting energies are very close to the previous ones, i. e. -19.24 MeV, -19.28 MeV and -19.25 MeV, but the basis sizes are almost doubled. To test the choice of ε, we made three calculations with $\varepsilon = 0.005$ MeV. The lowest calculated energy obtained is $E = -19.27$ MeV, in good agreement with the former calculations, but the basis sizes increased considerably ($N = 631$, $n = 193$).

We also calculated the spectroscopic (or formation) amplitude defined by

$$g(r) = \langle \Phi^{(r)} | \Psi_{00} \rangle, \tag{10}$$

with

$$\Phi^{(r)} = \Phi_\alpha \frac{\delta(r - r_{c\alpha})}{r_{c\alpha}} Y_{LM}(\hat{r}_{c\alpha}), \tag{11}$$

where Φ_α is the intrinsic wave function of the α particle constructed from a $0s$ harmonic-oscillator Slater determinant with size parameter ν_α. (See Ref. [1] for details.) The amplitudes of the present model and of the cluster-configuration shell model are compared in Fig. 2. The main peak is smaller and its position is somewhat closer to the origin (at 8.0 fm) in the present model than in the cluster-configuration model (8.2 fm).

The present spectroscopic factor is 0.011, while it is 0.023 in the hybrid model.

To calculate the decay width Γ, we use the R-matrix formula [9]

$$\Gamma = 2P(a) \frac{\hbar^2}{2M_\alpha a} g^2(a), \tag{12}$$

where M_α is the reduced mass, a is the channel radius and P is the Coulomb penetration factor. The width, calculated in the interval 10fm $\leq a \leq$ 12 fm, where the effect of the nuclear forces and Pauli exchanges are negligible, is $\Gamma = 7.2 \times 10^{-16}$ MeV. This value is about one third of the hybrid-model value ($\Gamma = 2.1 \times 10^{-15}$) and about one half of the experimental ($\Gamma = 1.5 \times 10^{-15}$) value. Note that the conventional shell model, like that of ref. [1], give much smaller and spacially confined amplitudes, while the shell models with sophisticated truncation schemes [10, 11] give amplitudes of comparable extensions but smaller spectroscopic factors and decay widths.

5 Summary

With the help of a stochastic variational method, a flexible shell-model wave function has been constructed for the g.s. of ^{212}Po using combinations of gaussian functions as s.p. orbits. The present model gives nearly as good a result for the α-decay width as our former cluster-configuration shell model, which is sharpened just to describe α-decay. The chief merit of the model presented here is its technical simplicity, which makes it easily applicable to other α-decays or even to heavy-cluster decays.

This work was supported by the OTKA grants (No. 3010 and F4348). We are grateful to Prof. R. G. Lovas for useful discussions.

References

[1] K. Varga, R. G. Lovas and R. J. Liotta, Phys. Rev. Lett. **69** (1992) 37
K. Varga, R. G. Lovas and R. J. Liotta, Nucl. Phys. **A550** (1992) 421

[2] K. Varga, Y. Suzuki and R. G. Lovas, Nucl. Phys **A**, in press

[3] H. Horiuchi, Suppl. of Prog. Theor. Phys. **62** (1977) 90.

[4] Y. Suzuki and K. Ikeda, Phys. Rev. **C38** (1988) 410

[5] H. De Raedt and M. Frick, Physics Reports **231** (1993) 109
W. von der Linden, Physics Reports **220** (1992) 55

[6] B. N. Parlett, The symmetric eigenvalue problem (Prentice-Hall, N. J., 1980)

[7] D. M. Brink and E. Boeker, Nucl. Phys. **A91** (1967) 1

[8] E. Rost, Phys. Lett. **B26** (1968) 184

[9] R. G. Thomas, Prog. Theor. Phys. **12** (1954) 253

[10] I.Tonozuka and A. Arima, Nucl. Phys. **A323** (1979) 45

[11] G. Dodig-Crnkovic, F. A. Janouch and R. J. Liotta, Nucl. Phys. **A501** (1989) 533

Figure captions

Figure 1 Convergence of the energy of ^{212}Po (g.s.) as a function of the basis dimension N.
Figure 2 Formation amplitude g(r) (eq. (10)) as a function of the distance between the decaying α-particle and the daughter nucleus ^{208}Pb (g.s.)

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